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EXTENDED BASIS SET CALCULATIONS
OF ATOMIZATION ENERGIES: COMPARISON
OF ISOGYRIC AND DIRECT RESULTS

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I. INTRODUCTION

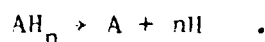
With the development of software efficiently implementing quantum chemical techniques that employ energy gradient and Hessian data, and the concurrent increase of access to modern supercomputers, systematic studies of molecular structures and properties have become routine. Recently, several groups have reported efforts to compute accurate values of molecular heats of formation. Pople and coworkers described a study of first-row hydrides using full fourth-order perturbation theory with a variety of basis sets.¹ In the same proceedings, Binkley and Frisch described results of perturbation theory studies of bond dissociation energies for a series of first-row diatomics.² The results described in these papers indicated that fourth-order perturbation theory calculations using extended basis sets provided generally excellent results for sigma-bonded systems, with less accurate results obtained for multiply bonded systems.

Subsequently, Page, et al., used a similar approach to evaluate the dimerization energy of borane.³ There were systematic differences among these studies that should be noted. Binkley and Frisch computed equilibrium structures using third-order perturbation theory, whereas the other calculations used structural parameters predicted at the Hartree-Fock level. Page, et al., employed an extended basis set when computing the energy, while the other authors approximated this extended basis set by assuming that the effects of individual basis set extensions were additive. Related to these efforts to predict molecular energies accurately, Handy and coworkers have published a series of papers that attempt to evaluate the success of various levels of theory in predicting the properties of molecules.^{4,5,6} Those computations all employed extended basis sets in order to isolate the effect of theoretical method from the effect of basis set deficiencies. This note describes the effects on computed atomization energies of variation in the theoretical model used to analyze extended basis set results. In particular, we focus on differences obtained when one uses either the isogyric analysis employed by Pople, et al.,¹ or the direct method of computation used in our previous reports.^{3,7} We also describe the application of isogyric analyses at several orders of perturbation theory.

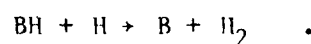
II. METHODS

We report a series of Moller-Plesset perturbation theory calculations on small molecules. These calculations employ large atomic centered basis sets for the expansion of the molecular orbitals, beginning with the 6-311G basis designed for use with correlation theory methods.⁸ This basis is augmented by including diffuse functions, s-type for hydrogen and both s- and p-type for the first row atoms. Additionally three sets of functions in the first polarization space and one set in the second polarization space are added for each atom. For the largest molecule studied, diborane, the total number of basis functions is 186. Perturbation theory calculations were performed using the GAUSSIAN82 computer programs⁹ for structures optimized at the SCF level using the well-known double zeta plus polarization basis set.^{10,11} Structures for those compounds characterized by open-shell wavefunctions were computed using unrestricted Hartree-Fock wavefunctions. Harmonic frequencies were also computed using SCF methods with the DZP basis.

Results are reported for all three B₁ hydrides and diborane, as well as water, ammonia, hydroxyl radical, carbon monoxide, boron oxide, BO, and methane. The atomization energies of the compounds are evaluated in two ways. One technique computes directly the difference between the sum of the energies of the constituent atoms and the molecule's energy. That is, we compute the energy for the process,



Alternately, we evaluate the energy using the isogyric technique described by Pople, et al., in Reference 1. In this case, energies relative to that of the hydrogen molecule are computed using reactions for which the number of unpaired spins is conserved. This is equivalent to conserving the number of electron pairs among the species involved in the comparison. Knowing the number of unpaired electrons for a particular atomic ground state enables one to write isogyric comparisons with molecular hydrogen. For the BH molecule, one has,



Assuming that theory can predict the energy of a reaction producing an atom plus hydrogen molecule(s), then the precisely known value of the dissociation energy for the H₂¹² can be used to give the value of D₀ for the molecule of interest.

Our computations differ from those of Pople, et al., in several ways. The theoretical energies used in their analysis were obtained by improving the results of energies computed using fourth-order Moller-Plesset theory with the 6-311G** basis set. Initially, they estimated a correction to the correlation energy by using an extrapolation method that estimates the contribution made by orders of perturbation greater than four. The extrapolation procedure produced atomization energies that differed little from the fourth-order results. In some cases, agreement with experiment was poorer, an indication that the main source of error was the incompleteness of the basis set used to describe the molecular orbitals. Additionally, the fourth-order perturbation theory calculations ignored the energy contribution due to excitations of the electrons in the 1s core of the first row atoms. Most of our calculations do not make this approximation, but neither do we employ the extrapolation procedure to estimate the energy contribution obtained, perhaps, at higher orders of perturbation theory.

The basis set improvements in Reference 1 were evaluated incrementally; the effects of adding diffuse functions, polarization functions, and functions in the second polarization space were assumed to be additive. In the present case, all calculations are done with the extended basis set. Pople, et al., concluded that the addition of diffuse functions and second polarization functions had marked effects on the atomization energy calculation, but the effects of the first polarization functions were primarily equal for the atoms and the molecules.¹ If the effects of the basis set extensions were truly orthogonal, those results should closely mimic the data described here. Since it is unlikely that there is no cooperative effect, our approach should lead to slight differences with the incremental results.

In addition to the full fourth-order perturbation theory calculations, the diborane calculations were performed using the frozen core approximation. In order to obtain an indication of the effect of this approximation on the computed atomization energy, we have computed energies for several species using both a full perturbation theory calculation and the frozen core approximation. In addition, we have included the third-order perturbation theory results for each species. We anticipate the application of lower order perturbation theory results for larger molecules using semiempirical correction factors. Our goal here is to provide data on the application of this more approximate level of theory using extended basis sets.

III. RESULTS

We summarize the results of the perturbation theory calculations in Table 1. Our experience with the boranes indicated that extended basis set calculations yielded atomization energy predictions at third-order that were nearly equal to the full fourth-order perturbation theory predictions. With the data presented in this table, we can compare the third-order and fourth-order results over a larger class of compounds.

Table 1. Electronic Energy Results (Hartrees)

Molecule	Hartree-Fock	MP3	SDTQ-MP4	SDTQ-MP4(FC)
H	-0.49981	-0.49981	-0.49981	
B	-24.53108	-24.60644	-24.61167	-24.59308
C	-37.69025	-37.79163	-37.79638	-37.77642
N	-54.39889	-54.52976	-54.53302	-54.51173
O	-74.80934	-74.98919	-74.99316	-74.97094
H ₂	-1.13275	-1.17027	-1.17178	
BH	-25.12930	-25.23876	-25.24484	
BH ₂	-25.75976	-25.87763	-25.88193	
BH ₃	-26.39969	-26.55272	-26.55784	-26.53676
CH ₄	-40.21259	-40.45285	-40.46095	-40.43767
NH ₃	-56.21978	-56.49086	-56.50067	-56.47654
H ₂ O	-76.05931	-76.35067	-76.36215	-76.33811
OH	-75.41932	-75.65542	-75.66215	
BO	-99.55687	-99.89308	-99.91786	
O ₂	-149.67687	-150.14865	-150.17612	
B ₂ H ₆	-52.83425	-53.13056		-53.14242

Table 2 contains the data on all ten molecules studied. Both direct and isogyric predictions are reported for each molecule. In every case, the isogyric computation of the atomization energy, scaling with the known atomization energy of the hydrogen molecule, predicts a larger atomization energy than does the direct method of computation. The difference between the direct and isogyric comparison is equal to a multiple of the difference between the calculated atomization energy of the hydrogen molecule and the known value that we employ in our scaling.

Data comparing the results of full fourth-order atomization energy predictions with those obtained using third-order perturbation theory are presented in Table 3. Both direct and isogyric results are considered. The MP3 results preserve the energy difference between the direct and isogyric methods, although the magnitudes are greater than those obtained using the fourth-order data. For the hydrogen containing molecules, the energy differences between the third- and fourth-order results are not dramatically large, nor is the direction of the energy change constant. For the BO and O₂ molecules, on the other hand, the energy differences are large. Since neither molecule's atomization reaction can be described in terms of the breaking of a series of sigma bonds, it is not surprising that the reduced treatment of electron correlation provided at the MP3 level leads to so different a result than the full MP4 calculation. Triple-excitation diagrams that occur first at fourth-order, are required to describe the dissociation of these multiply-bonded systems.

Table 2. MP4 Predictions of Atomization Energies (Units: Hartrees)

Molecule	Full MP4		Frozen Core MP4	
	Direct	Isogyric	Direct	Isogyric
BH	0.13336	0.13566	-----	-----
BH ₂	0.27064	0.27294	-----	-----
BH ₃	0.44674	0.45134	0.44425	0.44884
CH ₄	0.66233	0.66923	0.66201	0.66891
NH ₃	0.46822	0.47512	0.46538	0.47228
H ₂ O	0.36937	0.37397	0.36755	0.37215
OH	0.16918	0.17148	-----	-----
BO	0.31303	0.31523	-----	-----
O ₂	0.18980	0.19210	-----	-----
B ₂ H ₆	-----	-----	0.95740	0.96660

Table 3. Comparison of MP3 and MP4 Atomization Energies (Units: H)

Molecule	SDTO-MP4		MP3	
	Direct	Isogyric	Direct	Isogyric
BH	0.13336	0.13566	0.13251	0.13632
BH ₂	0.27064	0.27294	0.27157	0.27538
BH ₃	0.44674	0.45134	0.44685	0.45447
CH ₄	0.66233	0.66923	0.66198	0.67341
NH ₃	0.46822	0.47512	0.46167	0.47310
H ₂ O	0.36937	0.37397	0.36186	0.36948
OH	0.16918	0.17148	0.16642	0.17023
BO	0.31303	0.31533	0.29745	0.30126
O ₂	0.18980	0.19210	0.17027	0.17408

IV. DISCUSSION

Handy and coworkers in a series of publications investigated the effect of the level of correlation energy on the prediction of molecular structures and spectroscopic properties.^{4,5,6} Most of these studies used an extended basis set similar to that employed in this work. In each case, the rationale is that the extended basis set removes at least one variable from the analysis of the results; additional basis set improvements will have scant effect. We assume that this is so in our calculations. While we have not set out to determine the convergence of the perturbation sequence with respect to the atomization energy predictions, we can comment on that based upon the third-order perturbation theory results.

The most obvious characteristic of these calculations is the systematic difference in predicted atomization energy that occurs at each level of theory investigated. Isogyric analysis always predicts a larger atomization energy than does a direct computation, with the difference between the methods increasing as the completeness of the theoretical treatment of correlation is reduced. This must occur, since the magnitude of the correction factor increases as the level of sophistication of correlation energy calculation is reduced.

It is also true that the full fourth-order perturbation theory atomization energies always exceed the frozen core results. The differences are generally small, a consequence of the fact that all the cases for which we can compare numbers involve a single first-row atom. In addition, our frozen core predictions are always equal to or greater than the predictions given by Pople, et al., for the same molecules. These differences are primarily due to the difference in hydrogen atom basis sets used in the two sets of calculations.

As discussed previously, the difference between the direct calculation of the atomization energy and the isogyric prediction is a multiple of the difference between the computed energy for the hydrogen molecule and the exact value. Thus, the correction factor for the BH molecule is one-third that of the methane molecule. To evaluate the results of the calculations, we compare the atomization energy predictions to those given in Reference 1. Those authors evaluated zero-point energy contributions using the best vibrational frequency data available at that time. There are cases, especially for the BH₂ molecule, the experimental numbers for both frequency and heat of formation are clearly incorrect. These empirically derived data, along with the results of our calculations and the frozen core data of Pople, et al., are summarized in Table 4. Note that the full MP4 calculations using the isogyric method of analysis overestimates the empirical atomization energy in every case but one, the BH₂ molecule. Our value for BH₃ is higher than that derived in a recent experimental study.¹⁴ That report assigns a D₀ value of 265.3 kcal/mole, from which we derive a D₀ equal to 280.6 kcal/mole, using our previously reported zero point energy.³ Our direct computation of the atomization energies tend to be close to the frozen core results, and are always lower than the experimental values, except for the BH molecule. In this case, there is reason to question the accuracy of the theoretical result. Both the BH molecule and the boron atom have low-lying excited states that are the consequence of double excitations. The perturbation theory techniques used in this study do not accurately account for the energy

contribution due to these excited states. Curtis and Pople have described a technique for computing corrections due to higher-order perturbation theory terms,¹⁵ and they have demonstrated the application of the technique in a study of small boron compounds.¹⁶ That analysis leads to a reduction by several kcal/mole of the atomization energies originally reported in Reference 1.

Since the magnitudes of the energy differences between theory and experiment are so small it is not possible to assign the "correct" value, except in the case of BH_2 for which the empirical value is known to be incorrect.

Table 4. Theoretical and Experimental Atomization Energies (kcal/mole)

Molecule	SDTQ-MP4		MP3	SDTQ-MP4-FC ¹	Experiment ¹³
	Direct	Isogyric			
BH	83.7	85.1	85.5	85.3	82.8
BH_2	169.8	171.2	172.8	168.5	196.2
BH_3	280.3	283.2	285.2	280.9	280.6 ¹⁴
CH_4	415.6	419.8	422.5	419.9	419.8
NH_3	293.8	298.1	296.9	296.2	297.3
H_2O	231.8	234.7	231.8	230.9	232.2
OH	106.2	107.6	106.9	105.5	106.6

Finally, we consider results of the isogyric analysis with the third-order perturbation theory results. As noted above, this technique fails utterly when applied to multiply bonded systems. In the case of the hydrides, however, the large basis set predictions are in reasonable agreement with the full fourth-order results. In every case, the corrected third order results exceed the atomization energy predictions of the direct calculations and the frozen-core calculations. There is not a systematic difference between the third- and fourth-order isogyric results, however. While admitting that the test set is small, we must conclude that the third-order perturbation theory calculations do provide surprisingly reasonable values for the sigma bonded molecules. Certainly, a more thorough evaluation of the application of extended basis set third-order results for sigma bonded systems seems warranted, since the computational advantages of this lower level of theory are substantial. The recent description of Carter and Goddard of an excellent prediction of the methylene singlet-triplet splitting obtained using an extended basis set with the computationally efficient GVB method¹⁷ also indicates the potential benefits of this genre of quantum chemical technique.

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